Neural Path Features and Neural Path Kernel : Understanding the role of gates in deep learning

Abstract

Rectified linear unit (ReLU) activations can also be thought of as *gates*, which, either pass or stop their pre-activation input when they are *on* (when the pre-activation input is positive) or *off* (when the pre-activation input is negative) respectively. A deep neural network (DNN) with ReLU activations has many gates, and the on/off status of each gate changes across input examples as well as network parameters. For a given input example, only a subset of gates are *active*, i.e., on, and the sub-network of weights connected to these active gates is responsible for producing the output. While at randomised initialisation, the active sub-network corresponding to a given input example is random, during training, as the network parameters are learnt, the sub-network is also learnt, and potentially holds very valuable information.

Our aim is to understand the role of the gates, and the dynamics of gate activity during training in DNNs. In this paper, we encode the on/off state of the gates of a given input in a novel *neural path feature* (NPF), and the weights of the DNN are encoded in a novel *neural path value* (NPV). Further, we show that the output of network is indeed the inner product of NPF and NPV. The main result of the paper shows that the *neural path kernel* associated with the NPF is a fundamental quantity that characterises the information stored in the gates of a DNN. We show via experiments (on MNIST and CIFAR-10) that in standard DNNs with ReLU activations NPFs are learnt during training and such learning is key for generalisation. Furthermore, NPFs and NPVs can be learnt in two separate networks and such learning also generalises well in experiments. In our experiments, we observe that almost all the information learnt by a DNN with ReLU activations is stored in the gates - a novel observation that underscores the need to further investigate the role of gating in DNNs.

1 Introduction

We consider deep neural networks (DNNs) with rectified linear unit (ReLU) activations. A special property of ReLU activations is that they can also be thought of as *gates*, which are $1/0$ (i.e., on/off) depending on whether or not their pre-activation input is positive or negative. While the weights remain the same across input examples, the $1/0$ state of the gates change across input examples. For each input example, there is a corresponding *active* sub-network consisting of those gates which are 1, and the weights which pass through such gates. This active sub-network can be said to hold the memory for a given input, i.e., only those weights that pass through such active gates contribute to the output. In this viewpoint, at random initialisation of the weights, for a given input example, a random sub-network is active and produces a random output. However, as the weights change during training (say via gradient descent), the $1/0$ states of the gates, and hence the active sub-networks corresponding to the various input examples also change. At the end of training, for each input example, there is a learned active sub-network, and produces a learned output. Thus, the gates of a trained DNN could potentially contain valuable information.

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In this paper, we study the role of the gates, and the dynamics of the gates, i.e., the change in the states of the gates while training DNNs using gradient descent (GD). Our findings can be summarised in the following claims which we theoretically/experimentally justify in the paper:

Claim I (see Section 6): *Active sub-network are fundamental entities in DNNs.*

Claim II(see Section 5): *Active sub-networks are learnt during training via GD.*

Before we discuss "Claims I and II" in terms of the novel contributions in this paper in Section 1.2, we present the background of *neural tangent feature and kernel* (NTF and NTK) in Section 1.1.

Notation: We consider fully-connected DNNs with w hidden units per layer and $d-1$ hidden layers. The DNN accepts an input $x \in \mathbb{R}^{d_{in}}$ and produces an output $\hat{y}_\Theta(x) \in \mathbb{R}$, where $\Theta \in \mathbb{R}^{d_{net}}$ are the network weight ($d_{net} = d_{in}w + (d-2)w^2 + w$). We denote by $\Theta(l,j,i)$, the weight connecting the j^{th} hidden unit of layer $l-1$ to the i^{th} hidden unit of layer $l \in [d]$. $\Theta(1) \in \mathbb{R}^{w \times d_{in}}, \Theta(l) \in \mathbb{R}^{w \times w}, \forall l \in \{2,\ldots,d-1\}, \Theta(d) \in \mathbb{R}^{w \times 1}$. The dataset is given by $(x_s, y_s)_{s=1}^n \in \mathbb{R}^{d_{in}} \times \mathbb{R}$. The loss function is given by $L_\Theta = \frac{1}{2}\sum_{s=1}^n \left(\hat{y}_\Theta(x_s) - y_s\right)^2$. We consider the gradient descent update given by $\Theta_t = \Theta_t - \alpha_t(\nabla_\Theta L_{\Theta_t})$, where $\alpha_t > 0$ is a small step-size and $\nabla_\Theta(\cdot)$ stands for the gradient of $(\cdot)$ with respect to the network weights. We denote the set $\{1,\ldots,n\}$ by $[n]$. We use vectorised notations $y = (y_s, s \in [n]), \hat{y}_\Theta = (\hat{y}_\Theta(x_s), s \in [n]) \in \mathbb{R}^n$ for the true and predicted outputs and $e_t = (\hat{y}_{\Theta_t} - y) \in \mathbb{R}^n$ for the error in the prediction. We use θ to denote single arbitrary weight, and $\partial_\theta(\cdot)$ to denote $\frac{\partial(\cdot)}{\partial\theta}$.

1.1 Background: Neural Tangent Feature and Kernel

The NTF and NTK machinery was developed in some of the recent works [4, 1, 2, 3] to understand optimisation and generalisation in DNNs trained using GD. For an input $x \in \mathbb{R}^{d_{in}}$, the NTF is given by $\psi_{x,\Theta} = \nabla_\Theta \hat{y}_\Theta(x) \in \mathbb{R}^{d_{net}}$, i.e., the gradient of the network output with respect to its weights. The NTK matrix on the dataset is the $n \times n$ Gram matrix of the NTFs of the input examples, and is given by $K_\Theta(s,s') = \langle \psi_{x_s,\Theta}, \psi_{x_{s'},\Theta} \rangle, s, s' \in [n]$.

Proposition 1.1 (**Lemma 3.1** Arora et al. [2019]). *Consider the GD procedure to minimise the the squared loss $L(\Theta)$ the infinitesimally small step-size: $\dot{\Theta}_t = -\nabla_\Theta L_{\Theta_t}$. If follows that the dynamics of the error term can be written as $\dot{e}_t = -K_{\Theta_t} e_t$.*

Prior works [4, 3, 1, 2] have studied DNNs trained using GD in the so called 'NTK regime', which occurs under appropriate randomised initialisation, and when the width of the DNN approaches infinity. The characterising property of the NTK regime is that as $w \to \infty$, $K_{\Theta_0} \to K^{(d)}$, and $K_{\Theta_t} \approx K^{(d)}$, where $K^{(d)}$ (see (4) in Appendix A) is a deterministic matrix whose superscript (d) denotes the depth of the DNN. Arora et al. [2019] show that infinite width DNN trained using GD is equivalent to kernel regression with the limiting NTK matrix $K^{(d)}$ (and hence enjoys the generalisation ability of the limiting NTK matrix $K^{(d)}$). Further, Arora et al. [2019] propose a pure kernel method based on what they call the CNTK, which is the limiting NTK matrix $K^{(d)}$ for an infinite width convolutional neural network (CNN). Cao and Gu [2019] show that in the NTK regime, a DNN is almost a linear learner with the random NTFs at initialisation, and showed a generalisation bound in the form of $\tilde{\mathcal{O}}\left(d \cdot \sqrt{y^\top \left(K^{(d)}\right)^{-1} y/n}\right)$[1].

Open Question: Arora et al. [2019] report a $5\% - 6\%$ performance gap between exact CNTKs corresponding to infinite width CNNs and finite width CNNs (which do not operate in the NTK regime). Based on this performance gap they infer that finite width is beneficial and and that the study of DNNs in the NTK regime cannot fully explain the success of practical neural networks yet.

1.2 Our Contributions

• **Gate Encoding (Section 2):** We encode the states of the gates in a novel *neural path feature* (NPF) and the weights in a novel *neural path value* (NPV) and express the output of the DNN as an inner product of NPF and NPV. In contrast to NTF/NTK which are *first-order* quantities (based on derivatives with respect to the weights), NPF and NPV are *zeroth-order* quantities.

[1] $a_t = \mathcal{O}(b_t)$ if $\limsup_{t\to\infty} |a_t/b_t| < \infty$, and $\tilde{\mathcal{O}}(\cdot)$ is used to hide logarithmic factors in $\mathcal{O}(\cdot)$.

• **Gate Dynamics (Section 3):** In the case of a ReLU gate with pre-activation $q \in \mathbb{R}$, the '$1/0$' state of the gate is given by $\gamma_r(q) = \mathbb{1}_{\{q>0\}}$, whose derivative $\frac{d\gamma_r(q)}{dq} = 0$ almost everywhere. Thus, the sensitivity of the state of the gates to the DNN weights is not accounted in the NTF/NTK expressions in prior works. We use 'soft-ReLU' given by $\gamma_{sr}(q) = \frac{1}{(1+\exp(-\beta \cdot q))}, \beta > 0$, which is differentiable with respect to q and capture the changes in the state of the gates, i.e., change of the NPFs during GD.

• **Gate Decoupling (Section 4):** We introduce a deep gated network (DGN) framework, wherein, the NPF and the NPV are decoupled by storing them in two separate networks. This enables us to fix the NPFs during training (i.e., keep them constant) and learn only the NPVs via GD, and measure the information stored in the gates/NPFs. We also use the DGN framework to learn NPFs and NPV in a 'decoupled' manner using two separate set of weights, and demonstrate the power of NPF learning.

• **Interpretable Kernel (Section 5):** We show that in the case of training with fixed NPFs, in the limit of infinite width, the NTK matrix can be simplified and the NTK is equal to the NPK times a constant (see Theorem 5.1). The fixed NPF setting needs tighter assumptions (Assumption 5.1) than the prior works on NTK. However, what we lose in generality, we gain in *interpretability*. The NPK can be decomposed as a *Hadamard* product of the input Gram matrix, and a correlation matrix of active sub-networks. Thus the information stored in the gates/NPFs is characterised in terms of the active sub-networks. This justifies our "Claim I".

• **NPF Learning (Section 6) :** We show that in finite width DNNs with ReLU activations, NPFs are learnt continuously during training, and such learning is key for generalisation. We observe that fixed NPFs obtained from the initial stages of training generalise poorly than CNTK (of Arora et al. [2019]), whereas, fixed NPFs obtained from later stages of training generalise better than CNTK and generalise as well as standard DNNs with ReLU. This throws light on the open question in Section 1.1, i.e., the difference between the NTK regime and the finite width DNNs is perhaps due to NPF learning. In finite width DNNs, NPFs are learnt during training and in the NTK regime no such feature learning happens during training (since $K^{(d)}$ is fixed). This justifies our "Claim II".

2 Neural Path Feature and Kernel: Encoding Gating Information

The gating property of the ReLU activation allows us to express the output of the network as a summation of the contribution of the individual paths, and paves a natural way to encode the $1/0$ states of the gates *without loss of information*. The contribution of a path is the product of the signal in its input node, the 'd' weights in the path and the '$(d-1)$' gates in the path. For an input $x \in \mathbb{R}^{d_{in}}$, and parameter $\Theta \in \mathbb{R}^{d_{net}}$, we encode the gating information in a novel *neural path feature* (NPF), $\phi_{x,\Theta} \in \mathbb{R}^P$ and the weights in a novel *neural path value* (NPV) $v_\Theta \in \mathbb{R}^P$, where, $P = d_{in} w^{(d-1)}$ is the total number of paths. The NPF co-ordinate of a path is the product of the signal at its input node and the gates in the path. The NPV co-ordinate of a path is the product of the weights in the paths. By stacking the NPFs of all the input examples we obtain the NPF matrix as $\Phi_\Theta = (\phi_{x_s,\Theta}, s \in [n]) \in \mathbb{R}^{P \times n}$. Then the input-output relationship of a DNN in vector form is given by:

$$\hat{y}_\Theta = \Phi_\Theta^\top v_\Theta, \tag{1}$$

where the NPF matrix Φ_Θ can also be interpreted as the *hidden feature matrix* which along with v_Θ is learnt during gradient descent on $\Theta \in \mathbb{R}^{d_{net}}$.

2.1 Paths

Input Layer	$z_{x,\Theta}(0)$	$=$	x
Pre-Activation	$q_{x,\Theta}(l,i)$	$=$	$\Theta(l,\cdot,i)^\top z_{x,\Theta}(l-1), l \in [d-1], i \in [w]$
Gating Values	$G_{x,\Theta}(l,i)$	$=$	$\gamma_r(q_{x,\Theta}(l,i)), l \in [d-1], i \in [w]$, where $\gamma_r(q) = \mathbb{1}_{\{q>0\}}$
Hidden Layer	$z_{x,\Theta}(l,i)$	$=$	$\chi_r(q_{x,\Theta}(l,i)) = q_{x,\Theta}(l,i) \cdot G_{x,\Theta}(l,i), l \in [d-1], i \in [w]$
Final Output	$\hat{y}_\Theta(x)$	$=$	$\Theta(d)^\top z_{x,\Theta}(d-1)$

Table 1: DNN with ReLU activation $\chi_r(q) = q \cdot \gamma_r(q)$, where $\gamma_r(q) = \mathbb{1}_{\{q>0\}}$ is the ReLU gate.

A path starts from an input node, passes through exactly one weight (and one hidden node) in each layer and ends at the output node. We have a total of $P = d_{in} w^{(d-1)}$ paths. Let us say that an enumeration of the paths is given by $[P]=\{1,\dots,P\}$. Let $\mathcal{I}_l\colon[P]\to[w], l=0,\dots,d-1$ provide the index of the hidden unit through which a path p passes in layer l (with the convention that $\mathcal{I}_d(p)=1,\forall p\in[P]$).

2.2 Neural Path Feature, Neural Path Value and Network Output

Definition 2.1. *Let $x\in\mathbb{R}^{d_{in}}$ be the input to the DNN. For this input,*

(i) The activity of a path p is given by : $A_\Theta(x,p)\stackrel{def}{=}\Pi_{l=1}^{d-1}G_{x,\Theta}(l,\mathcal{I}_l(p))$.

(ii) The neural path feature (NPF) is given by : $\phi_{x,\Theta}\stackrel{def}{=}(x(\mathcal{I}_0(p))A_\Theta(x_s,p),p\in[P])\in\mathbb{R}^P$.

(iii) The neural path value (NPV) if given by : $v_\Theta\stackrel{def}{=}\left(\Pi_{l=1}^{d}\Theta(l,\mathcal{I}_{l-1}(p),\mathcal{I}_l(p)),p\in[P]\right)\in\mathbb{R}^P$.

A path p is active if all the gates in the paths are on.

Proposition 2.1. *In DNNs without any bias, the NPFs are* positively homogeneous, *i.e.,* $\phi_{cx,\Theta}=c\phi_{x,\Theta},\forall c>0,x\in\mathbb{R}^{d_{in}}$.

Proposition 2.2. *The output of the network can be written as an inner product of the NPF and NPV, i.e.,* $\hat{y}_\Theta(x)=\langle\phi_{x,\Theta},v_\Theta\rangle=\sum_{p\in[P]}x(\mathcal{I}_0(p))A_\Theta(x,p)v_\Theta(p)$.

2.3 Neural Path Kernel : Similarity based on active sub-networks

The NPK is defined as $H_\Theta\stackrel{def}{=}\Phi_\Theta^\top\Phi_\Theta$.

Definition 2.2. *For input examples $s,s'\in[n]$ define*

1. $\tau_\Theta(s,s',l)\stackrel{def}{=}\sum_{i=1}^{w}G_{x_s,\Theta}(l,i)G_{x_{s'},\Theta}(l,i)$ *be the number of activations that are "on" for both inputs $s,s'\in[n]$ in layer $l\in[d-1]$.*

2. $\Lambda_\Theta(s,s')\stackrel{def}{=}\Pi_{l=1}^{d-1}\tau_\Theta(s,s',l)$.

For a given example $s\in[n]$, $\Lambda_\Theta(s,s)$ is a measure of the total number of active paths for that input example, and for different input examples $s,s'\in[n]$ it is a measure of total number of paths that are active for both examples $s,s'\in[n]$. Thus, $\Lambda_\Theta\in\mathbb{R}^{n\times n}$ is the correlation matrix that measures the amount of overlap the active sub-networks.

Lemma 2.1. *Let $\Sigma\in\mathbb{R}^{n\times n}$ be the $n\times n$ input Gram matrix with $\Sigma(s,s')=\langle x_s,x_{s'}\rangle, s,s'\in[n]$. It follows that $H_\Theta=\Sigma\odot\Lambda_\Theta$, where $\odot$ stands for the Hadamard product.*

3 Dynamics of Gradient Descent with NPF and NPV Learning

In this section, in addition to the dynamics of the weights, and the error term (as in Proposition 1.1), we also capture the dynamics of the NPF and the NPV learning during GD.

3.1 Expanding Neural Tangent Features and Neural Tangent Kernel

By 'plugging' the expression for $\hat{y}_\Theta(x)$ in $\partial_\theta\hat{y}_\Theta(x)$, we have

$$\begin{aligned}\partial_\theta\hat{y}_\Theta(x)&=\underbrace{\langle\phi_{x,\Theta},\partial_\theta v_\Theta\rangle}_{\text{value derivative}}+\underbrace{\langle\partial_\theta\phi_{x,\Theta},v_\Theta\rangle}_{\text{feature derivative}}\\&=\sum_{p\in[P]}x(\mathcal{I}_0(p))A_\Theta(x,p)\partial_\theta v_\Theta(p)+\sum_{p\in[P]}x(\mathcal{I}_0(p))\partial_\theta A_\Theta(x,p)v_\Theta(p)\end{aligned}\tag{2}$$

Note that due to the $A_\Theta(x,p)$, only active paths (those passing through active gates) contribute to the value derivative, and due to the $\partial A_\Theta(x,p)$, only sensitive paths (those passing through sensitive gates) contribute to the feature derivative. The next two results Propositions 3.1 and 3.2 characterise the $\partial_\theta v_\Theta(p)$ and the $\partial_\theta A_\Theta(x,p)$ terms.

Proposition 3.1. *Let p be a path, and let $\theta\in\Theta$ be an arbitrary weight belonging to layer $l'\in[d]$ such that $\theta=\Theta(l',i,j)$. Then $\partial_\theta v_\Theta(p)=0$ if the path does not pass through the weight, and* $\partial_\theta v_\Theta(p)=\Pi_{l\neq l',l=1}^{d}\Theta(l,\mathcal{I}_{l-1}(p),\mathcal{I}_l(p))$.

Proposition 3.2. *Let p be a path, and let $\theta \in \Theta$ be an arbitrary weight, then $\partial_\theta A_\Theta(x,p) = \sum_{l=1}^{d} \partial_\theta G_{x,\Theta}(l) \Pi_{l' \neq l} G_{x,\Theta}(l')$.*

From (2) we have $\psi_{x,\Theta} = \psi^{\text{V}}_{x,\Theta} + \psi^{\text{F}}_{x,\Theta}$, where ψ^{V} and ψ^{F} denote the value and feature gradients given by $\psi^{\text{V}}_{x,\Theta} = (\langle \phi_{x,\Theta}, \partial_\theta v_\Theta \rangle, \theta \in \Theta) \in \mathbb{R}^{d_{net}}$ and $\psi^{\text{F}}_{x,\Theta} = (\langle \partial_\theta \phi_{x,\Theta}, v_\Theta \rangle, \theta \in \Theta) \in \mathbb{R}^{d_{net}}$ respectively. The NTK matrix is given by $K_\Theta(s,s') = \langle \psi_{x_s,\Theta}, \psi_{x_{s'},\Theta} \rangle$, $s, s' \in [n]$ and can be further decomposed as:

$$K_\Theta(s,s') = \underbrace{K^{\text{V}}_\Theta(s,s')}_{\langle \psi^{\text{V}}_{x_s,\Theta}, \psi^{\text{V}}_{x_{s'},\Theta} \rangle} + \underbrace{K^{\text{F}}_\Theta(s,s')}_{\langle \psi^{\text{F}}_{x_s,\Theta}, \psi^{\text{F}}_{x_{s'},\Theta} \rangle} + \underbrace{K^{\text{CROSS}}_\Theta(s,s')}_{\langle \psi^{\text{V}}_{x_s,\Theta}, \psi^{\text{F}}_{x_{s'},\Theta} \rangle + \langle \psi^{\text{F}}_{x_s,\Theta}, \psi^{\text{V}}_{x_{s'},\Theta} \rangle} \qquad (3)$$

3.2 Gradient Descent Dynamics in DNN with ReLU

An important point to note here is that the derivative of the ReLU gates (i.e., $1/0$ state) with respect to its pre-activation is almost surely 0. As a result, in (2) $\partial_\theta A_\theta(\cdot,\cdot) = 0$ and hence $\psi^{\text{F}}_{x,\Theta} = 0$, $K^{\text{F}}_\Theta = K^{\text{CROSS}}_\Theta = 0$. However, the NPF changes at those time instants when any one of the gates switches from 1 to 0 or from 0 to 1. In the time between two such switching instances, NPFs of all the input examples in the dataset remain the same, and between successive switching instances, the NPF of at least one of the input example in the dataset changes.

Definition 3.1. *Define a sequence of monotonically increasing time instants $\{T_i\}_{i=0}^{\infty}$ (with $T_0 = 0$) to be 'switching' instants if $\phi_{x_s,\Theta_t} = \phi_{x_s,\Theta_{T_i}}, \forall s \in [n], \forall t \in [T_i, T_{i+1}), i = 0, \ldots, \infty$, and $\forall i = 0, \ldots, \infty\ \exists s(i) \in [n]$ such that $\phi_{x_{s(i)},\Theta_{T_i}} \neq \phi_{x_{s(i)},\Theta_{T_{i+1}}}$.*

Proposition 3.3. *Let $\nabla_\Theta v_\Theta$ be a $P \times d_{net}$ matrix of NPV derivatives with entries $\nabla_\Theta v_\Theta(p,\theta) = \partial_\theta v_\Theta(p), \theta \in \Theta, p \in [P]$. Let the maximum and minimum eigenvalue of a real symmetric matrix A be $\rho_{\max}(A)$ and $\rho_{\min}(A)$.Then for $t \in [T_i, T_{i+1})$ and infinitesimally small step-size of GD:*

Weights	$\dot{\Theta}_t$	$=$	$-\sum_{s=1}^{n} \psi_{x_s,\Theta_t} e_t(s) = \sum_{s=1}^{n} (\psi^{\text{V}}_{x_s,\Theta_t}) e_t(s)$
NPV	$\dot{v}_{\Theta_t}(p)$	$=$	$\sum_{\theta \in \Theta} \partial_\theta v_{\Theta_t}(p) \dot{\theta}_t, \forall p \in [P]$
Error	$\dot{e}_t$	$=$	$-K_{\Theta_t} e_t$, where $K_{\Theta_t} = \Phi^\top_{\Theta_{T_i}} \left((\nabla_\Theta v_{\Theta_t})(\nabla_\Theta v_{\Theta_t})^\top \right) \Phi_{\Theta_{T_i}}$

Further $\rho_{min}(K_{\Theta_t}) \leq \rho_{\min}(H_{\Theta_{T_i}}) \rho_{\max}\left((\nabla_\Theta v_{\Theta_t})(\nabla_\Theta v_{\Theta_t})^\top \right)$.

Remark: Informally speaking, H_Θ will be ill-conditioned when there exists input examples $s, s' \in [n]$ in the dataset that are almost same, as a consequence of which the s^{th} and s'^{th} rows (as well as columns) of the symmetric matrices Σ and Λ_Θ are very close (due to the similarity in active sub-networks for the two inputs that are very close). This is quite intuitive, in that, the closer two inputs are, the closer are their NPFs, and it is harder to train the network to produce arbitrarily different outputs for such inputs that are very close to one another.

3.3 Gradient Descent Dynamics in DNN with Soft-ReLU

We remedy the non-differentiability of $1/0$ state of the gates by the use of *soft-ReLU* gates, where the gating and activations are given by $\gamma_{sr}(q) = \frac{1}{(1+\exp(-\beta \cdot q))}, \beta > 0$, and $\chi_{sr}(q) = q \cdot \gamma_{sr}(q)$ respectively. The derivative of soft-ReLU gating with respect to its pre-activation is given by $\partial_q \gamma_{sr}(q) = \frac{\beta}{(1+\exp(\beta \cdot q))(1+\exp(-\beta \cdot q))}$. The soft-ReLU gating is to be regarded as a 'trick' to analytically relax the $1/0$ state and track its change in a continuous manner.

Proposition 3.4. *For an infinitesimally small step-size of GD, the error dynamics of a DNN with soft-ReLU gates is given by:*

Weights	$\dot{\Theta}_t$	$=$	$-\sum_{s=1}^{n} \psi_{x_s,\Theta_t} e_t(s) = \sum_{s=1}^{n} (\psi^{\text{V}}_{x_s,\Theta_t} + \psi^{\text{F}}_{x_s,\Theta_t}) e_t(s)$
NPF	$\dot{\phi}_{x_s,\Theta_t}(p)$	$=$	$x(\mathcal{I}_0(p)) \sum_{\theta \in \Theta} \partial_\theta A_{\Theta_t}(x_s,p) \dot{\theta}_t, \forall p \in [P], s \in [n]$
NPV	$\dot{v}_{\Theta_t}(p)$	$=$	$\sum_{\theta \in \Theta} \partial_\theta v_{\Theta_t}(p) \dot{\theta}_t, \forall p \in [P]$
Error	$\dot{e}_t$	$=$	$-K_{\Theta_t} e_t$, where $K_\Theta = K^{\text{V}}_\Theta + K^{\text{F}}_\Theta + K^{\text{CROSS}}_\Theta$

Remark: Thanks to the soft-ReLU trick, we are able to capture the NPF learning via $\dot{\phi}_{x_s,\Theta_t}$ term.

4 Deep Gated Networks: Decoupling Neural Path Feature and Value

In order to ascertain that NPF learning indeed makes a difference, we should measure the generalisation performance with and without NPF learning. This can be achieved by a deep gated network (see Figure 1 below for details) having two networks of identical architecture namely i) a feature network parameterised by $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$, that holds gating information, and hence the NPFs and ii) a value network that holds the NPVs parameterised by $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$. By making $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ trainable/non-trainable, we can *enable/disable* the NPF gradient, which gives rise to the following two modes of operating a DGN:

1. **Fixed NPF (FNPF):** Here, $\Theta^{\text{F}}_t = \Theta^{\text{F}}_0, \forall t \geq 0$, i.e., $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ is non-trainable. Thus the DGN learns the relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi^\top_{\Theta^{\text{F}}_0} v_{\Theta^{\text{V}}}$, where $\Phi_{\Theta^{\text{F}}_0} \in \mathbb{R}^{P \times n}$ is a fixed NPF matrix, and $v_{\Theta^{\text{V}}}$ is learned via gradient descent on $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$.

2. **Decoupled NPF Learning (DNPFL):** Here both $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ and $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$ are trained, and the DGN learns the relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi^\top_{\Theta^{\text{F}}} v_{\Theta^{\text{V}}}$. In comparison to (1), here we have two parameters $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ and $\Theta^{\text{V}} \in \mathbb{R}^{d_{net}}$ as opposed to a single $\Theta \in \mathbb{R}^{d_{net}}$ in (1).

Note: FNPF and DNPFL are idealised modes to understand the role of gates, and not alternate proposals to replace standard DNNs with ReLU activations.

Layer	Feature Network (NPF)	Value Network (NPV)
Input	$z^{\text{F}}_{x,t}(0) = x$	$z^{\text{V}}_{x,t}(0) = x$
Activation	$q^{\text{F}}_{x,t}(l) = \Theta^{\text{F}}_t(l)^\top z^{\text{F}}_{x,t}(l-1)$	$q^{\text{V}}_{x,t}(l) = \Theta^{\text{V}}_t(l)^\top z^{\text{V}}_{x,t}(l-1)$
Hidden	$z^{\text{F}}_{x,t}(l) = \chi^{\text{F}}\left(q^{\text{F}}_{x,t}(l)\right)$	$z^{\text{V}}_{x,t}(l) = q^{\text{V}}_{x,t}(l) \odot G_{x,t}(l)$
Output	None	$\hat{y}_t(x) = \Theta^{\text{V}}(d)^\top z^{\text{V}}_{x,t}(d-1)$
Gating Values: $G_{x,t}(l) = \gamma_r\left(q^{\text{F}}_{x,t}(l)\right)$ or $G_{x,t}(l) = \gamma_{sr}\left(q^{\text{F}}_{x,t}(l)\right)$		

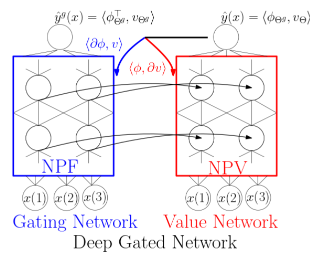

Figure 1: Deep gated network (DGN) setup. The pre-activations $q^{\text{F}}_{x,t}(l)$ of layer $l \in [d-1]$ from the feature network are used to derive the gating values $G_{x,t}(l)$ of layer $l \in [d-1]$.

Proposition 4.1 (DGN)**.** *Let $\psi^F_{x,\Theta^{DGN}} \stackrel{def}{=} \nabla_{\Theta^F} \hat{y}_{\Theta^{DGN}}(x) \in \mathbb{R}^{d_{net}}$, $\psi^V_{x,\Theta^{DGN}} \stackrel{def}{=} \nabla_{\Theta^V} \hat{y}_{\Theta^{DGN}}(x) \in \mathbb{R}^{d_{net}}$. For infinitesimally small step-size of GD, the error dynamics in a DGN (in the DNPFL and FNPF modes) is given by:*

			DNPFL	FNPF
Weight	$\dot{\Theta}^{\text{V}}_t$	$=$	$-\sum_{s=1}^n \psi^{\text{V}}_{x,\Theta^{\text{DGN}}_t} e_t(s)$, $\dot{\Theta}^{\text{F}}_t = -\sum_{s=1}^n \psi^{\text{F}}_{x,\Theta^{\text{DGN}}_t} e_t(s)$	$\dot{\Theta}^{\text{V}}_t$ same as (DNFPL), $\dot{\Theta}^{\text{F}}_t = 0$
NPF	$\dot{\phi}_{x_s,\Theta^{\text{F}}_t}(p)$	$=$	$x(\mathcal{I}_0(p)) \sum_{\theta^{\text{F}} \in \Theta^{\text{F}}} \partial_{\theta^{\text{F}}} A_{\Theta^{\text{F}}_t}(x_s, p) \dot{\theta}^{\text{F}}_t, \forall p \in [P], s \in [n]$	$\dot{\phi}_{x_s,\Theta^{\text{F}}_t}(p) = 0$
NPV	$\dot{v}_{\Theta^{\text{V}}_t}(p)$	$=$	$\sum_{\theta^{\text{V}} \in \Theta^{\text{V}}} \partial_{\theta^{\text{V}}} v_{\Theta^{\text{V}}_t}(p) \dot{\theta}^{\text{V}}_t, \forall p \in [P]$	$\dot{v}_{\Theta^{\text{V}}_t}(p)$ same as DNPFL
Kernel	$K_{\Theta^{\text{DGN}}}$	$=$	$K^{\text{V}}_{\Theta^{\text{DGN}}} + K^{\text{F}}_{\Theta^{\text{DGN}}}$	$K_{\Theta^{\text{DGN}}} = K^{\text{V}}_{\Theta^{\text{DGN}}}$
Error	$\dot{e}_t$	$=$	$-\left(K_{\Theta^{\text{DGN}}_t}\right) e_t$	$\dot{e}_t = -\left(K_{\Theta^{\text{DGN}}_t}\right) e_t$

Remark: The gradient dynamics in a DGN specified in Proposition 4.1 is similar to the gradient dynamics in a DNN specified in **??**. Important difference is that in a DGN there are $2d_{net}$ parameters, that value gradient $\psi^{\text{V}}_{x,\Theta^{\text{DGN}}}$ flows through the value network and the feature gradient $\psi^{\text{F}}_{x,\Theta^{\text{DGN}}}$ flows through the feature network. As a result $K^{\text{CROSS}}_{\Theta} = 0$. Note that in the FNPF mode of the DGN, since $\Theta^{\text{F}} \in \mathbb{R}^{d_{net}}$ are non-trainable $\psi^{\text{F}} = 0$, and hence $\dot{\phi} = 0$ and $K^{\text{F}}_{\Theta} = 0$.

5 Measure Of Gating Information and Neural Path Kernel

We now provide theoretical justification for "Claim I", i.e., the information in the gates of a DNN is captured in its active sub-networks. We define gating information as below.

Definition 5.1 (Measure of Gating Information)**.** *Define the measure of information stored in a* DNN *with parameter $\bar{\Theta} \in \mathbb{R}^{d_{net}}$ to be the generalisation performance of a* DGN *with identical architecture operated in the* FNPF *mode whose $\Theta^F_0 = \bar{\Theta}$ are non-trainable, and $\Theta^V \in \mathbb{R}^{d_{net}}$ are trained.*

Suppose we train a standard DNN for T epochs, and say the parameter at end of training is $\bar{\Theta}_T$. In this case, the relation learnt is $\hat{y}_{\bar{\Theta}_T} = \Phi_{\bar{\Theta}_T} v_{\bar{\Theta}_T}$. Thus, while measuring information in the gates of this trained DNN, as per Definition 5.1, we are retaining $\Phi_{\bar{\Theta}_T}$ by storing the weights as $\Theta^{\text{F}}_0 = \bar{\Theta}_T$ in the gating network, and discarding $v_{\bar{\Theta}_T}$, and re-training Θ^{V} to learn a new relation $\hat{y}_{\Theta^{\text{DGN}}} = \Phi_{\Theta^{\text{F}}_0} v_{\Theta^{\text{V}}} = \Phi_{\bar{\Theta}_T} v_{\Theta^{\text{V}}}$.

Assumption 5.1. *(i) $\Theta^V_0 \in \mathbb{R}^{d_{net}}$ is statistically independent of the fixed NPFs (corresponding to $\Theta^F_0 \in \mathbb{R}^{d_{net}}$), (ii) Θ^V_0 are sampled i.i.d from symmetric Bernoulli over $\{-\sigma, +\sigma\}$.*

Remark: Thus at initialisation as per Assumption 5.1 the NPFs and NPV are statistically independent.

Theorem 5.1. *For $4d/w^2 < 1$, as $w \to \infty$, $K_{\Theta^{DGN}_0} \to K^{(d)}_{DGN} = d \cdot \sigma^{2(d-1)} H_{\Theta^F_0} = d \cdot \Sigma \odot \bar{\Lambda}_{\Theta^F_0}$, where $\bar{\Lambda}_{\Theta^F_0} = \sigma^{2(d-1)} \Lambda_{\Theta^F_0}$.*

• From previous results, Arora et al. [2019], Cao and Gu [2019], if follows that as $w \to \infty$, the optimisation and generalisation properties of the fixed NPF learner can be tied down to $K^{(d)}_{DGN}$ and hence $H_{\Theta^{\text{F}}_0}$ (treating $d\sigma^{2(d-1)}$ as a scaling factor). "Claim I" is justified by noting that the NPK can be written as a *Hadamard* product of the input data Gram matrix and a correlation matrix of active sub-networks.

• The reason for the difference between the NTK matrices $K^{(d)}$ in (4) and $K^{(d)}_{DGN}$ in Theorem 5.1 is due to Assumption 5.1. Note that at initialisation in a DNN with ReLU gates (parameterised by $\Theta \in \mathbb{R}^{d_{net}}$), both NPFs and NPV are generated with respect to the weights $\Theta \in \mathbb{R}^{d_{net}}$ of the DNN. As a result, in a DNN with ReLU gates, Assumption 5.1 will be violated, i.e., at initialisation the NPFs and NPV are not statistically independent. However, in a DGN since we are decoupling the NPF and NPV, it is straightforward to satisfy Assumption 5.1.

• In our experiments we choose $\sigma = \frac{2}{w}$. Informally speaking, for symmetric randomised initialisation of Θ^{F}_0, we expect $\frac{w}{2}$ gates to be on every layer, so $\sigma = \frac{2}{w}$ is a normalising choice, because, the diagonal entries of $\bar{\Lambda}_{\Theta^{\text{F}}_0}(s, s) \approx 1$ in this case.

• We discuss a more detailed version of Theorem 5.1 in the Appendix, where we discuss the role of width and depth on a pure memorisation task.

6 Experiments

In this section, we experimentally verify "Claim II", that is, dynamics of the gates is key for generalisation. We compare the performance of the following networks on standard MNIST and CIFAR-10 datasets: i) fixed random (FRNPF): in the DGN, we randomly initialise both $\Theta^{\text{F}}_0, \Theta^{\text{V}}_0$, make Θ^{F} *non-trainable* and train only Θ^{V} , ii) fixed learnt (FLNPF): we initialise Θ^{V}_0 randomly, and copy weights from a pre-trained ReLU network (of identical architecture) into Θ^{F}_0. Similar to FR case, Θ^{F} is non-trainable and only Θ^{V} is trained iii) decoupled earning (DNPFL): we randomly initialise both $\Theta^{\text{F}}_0, \Theta^{\text{V}}_0$, and train both Θ^{F} and Θ^{V}, iv) Standard ReLU (ReLU). The results of our experiments on CIFAR-10 (please look at the Table 2 for complete results in CIFAR-10 as well as MNIST) that supports "Claim II' can be summarised as below:

1. FRNPF trains and generalises (67.08%), but ReLU (80.43%) and DNPFL (77.12%) perform better. This clearly shows that dynamics in the gates is key for generalisation.

2. FLNPF with weights copied from a fully trained ReLU performs close to 79.68% which is almost as good as ReLU (80.43%). Since from Theorem 5.1 we know that the generalisation performance of the fixed NPF learner is characterised by its NPK, and the fact that FLNPF almost recovers the performance of ReLU, we observe that *almost all the information learnt by a standard ReLU DNN is stored in its gates.*

3. The NPFs are learnt continuously during the training, and the performance gap between FRNPF and ReLU is continuous. We trained a DNN with ReLU (parameterised by $\bar{\Theta}$) for 60 epochs, and we obtained 6 different weights at various *stages* of the training process. Stage 1: $\bar{\Theta}_{10}$, stage 2: $\bar{\Theta}_{20}$, stage 3: $\bar{\Theta}_{30}$, stage 4: $\bar{\Theta}_{40}$, stage 5: $\bar{\Theta}_{50}$, stage 6: $\bar{\Theta}_{60}$. We copy these weights obtained at various stages of training to setup 6 different FLNPFs, i.e., FLNPF-1 to FLNPF-6. We observe that the performance of FLNPF-1 to FLNPF-6 increases monotonically, with FLNPF-1 performing 72%

which is better than FRNPF (i.e., 67.08%), and FLNPF-6 performing as well as ReLU (see Figure 2). The performance of the Convolutional NTK based pure kernel method in Arora et al. [2019] is 77.43%. Thus through its various stages, the FLNPF starts from below 77.43% and surpasses to reach 79.68%, which implies the difference in performance is clearly coming from learning of NPFs.

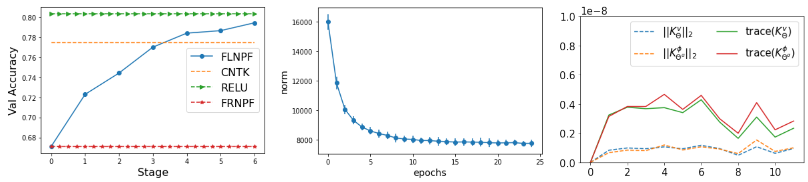

Figure 2: Dynamics of Learning

NPK during training: We considered "Binary"-MNIST data set with two classes namely digits 4 and 7, with the labels taking values in $\{-1,+1\}$ and squared loss. We trained a standard DNN with ReLU activation ($w=100$, $d=5$). Let $\widehat{H}_t = \frac{1}{trace(H_t)} H_t$ be the normalised NPK matrix. For a subset size, $n'=200$ (100 examples per class) we plot $\nu_t = y^\top(\widehat{H}_t)^{-1}y$, (where $y\in\{-1,1\}^{200}$ is the labelling function), and observe that ν_t reduces as training proceeds (see middle plot in Figure 2). Note that, $\nu_t=\sum_{i=1}^{n'}(u_{i,t}^\top y)^2(\hat{\rho}_{i,t})^{-1}$, where $u_{i,t}\in\mathbb{R}^{n'}$ are the orthonormal eigenvectors of $\widehat{H}_t$ and $\hat{\rho}_{i,t}, i\in[n']$ are the corresponding eigenvalues. Since $\sum_{i=1}^{n'}\hat{\rho}_{i,t}=1$, the only way ν_t reduces is when more and more energy gets concentrated on $\hat{\rho}_{i,t}$s for which $(u_{i,t}^\top y)^2$s are also high.

Role of K^{V}_{Θ} and K^{F}_{Θ}: In this case the of decoupled learning, NTK is given by $K_{\Theta^{\text{DGN}}} = K^{\text{V}}_{\Theta^{\text{DGN}}} + K^{\text{F}}_{\Theta^{\text{DGN}}}$. For MNIST, we compared $K^{\text{V}}_{\Theta^{\text{DGN}}}$ and $K^{\text{F}}_{\Theta^{\text{DGN}}}$ using their trace and Frobenius norms, and we observe that K^{v}_{Θ} and $K^{\phi}_{\Theta^{\text{F}}}$ are in the same scale, which is perhaps pointing to the fact that both K^{v}_{Θ} and $K^{\phi}_{\Theta^{\text{F}}}$ are equally important for obtaining good generalisation performance.

7 Conclusion and Future Work

Gradient is a first-order information, and learning with GD is essentially a process of integration, and naturally its outcome is a zeroth-order information. It turns out the NPFs capture this zeroth-order information, and plays a critical role in DNNs. We conclude by saying *understanding deep learning requires understanding NPF learning*. The DGN might be useful in this effort, since the NPFs learning is decoupled and is perhaps easier to analysis than standard DNNs.

References

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Arch	Optimiser	Dataset	FRNPF (II)	FRNPF (DI)	DNPFL	FLNPF	ReLU
FC	SGD	MNIST	95.85 ± 0.10	95.85 ± 0.17	97.86 ± 0.11	97.10 ± 0.09	97.85 ± 0.09
FC	Adam	MNIST	96.02 ± 0.13	96.09 ± 0.12	$\mathbf{98.22\pm0.05}$	$\mathbf{97.82\pm0.02}$	$\mathbf{98.14\pm0.07}$
VCONV	SGD	CIFAR-10	58.92 ± 0.62	58.83 ± 0.27	63.21 ± 0.07	63.06 ± 0.73	67.02 ± 0.43
VCONV	Adam	CIFAR-10	64.86 ± 1.18	64.68 ± 0.84	$\mathbf{69.45\pm0.76}$	$\mathbf{71.4\pm0.47}$	$\mathbf{72.43\pm0.54}$
GCONV	SGD	CIFAR-10	67.36 ± 0.56	66.86 ± 0.44	$\mathbf{74.57\pm0.43}$	$\mathbf{78.52\pm0.39}$	$\mathbf{78.90\pm0.37}$
GCONV	Adam	CIFAR-10	67.09 ± 0.58	67.08 ± 0.27	$\mathbf{77.12\pm0.19}$	$\mathbf{79.68\pm0.32}$	$\mathbf{80.43\pm0.35}$

Table 2: Shows the training and generalisation performance of various NPFs.

Arthur Jacot, Franck Gabriel, and Clément Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In *Advances in neural information processing systems*, pages 8571–8580, 2018.

8 Related Work

Appendix

A Expression for $K^{(d)}$

The $K^{(d)}$ matrix is computed by the recursion in (4).

$$\tilde{K}^{(1)}(s,s')=\Sigma^{(1)}(s,s')=\Sigma(s,s'), M^{(l)}_{ss'}=\begin{bmatrix}\Sigma^{(l)}(s,s) & \Sigma^{(l)}(s,s')\\ \Sigma^{(l)}(s',s) & \Sigma^{(l)}(s',s')\end{bmatrix}\in\mathbb{R}^2, \tag{4}$$

$$\Sigma^{(l+1)}(s,s')=2\cdot\mathbb{E}_{(q,q')\sim N(0,M^{(l)}_{ss'})}\left[\chi(q)\chi(q')\right], \hat{\Sigma}^{(l+1)}(s,s')=2\cdot\mathbb{E}_{(q,q')\sim N(0,M^{(l)}_{ss'})}\left[\partial\chi(q)\partial\chi(q')\right],$$

$$\tilde{K}^{(l+1)}=\tilde{K}^{(l)}\odot\hat{\Sigma}^{(l+1)}+\Sigma^{(l+1)}, K^{(d)}=\left(\tilde{K}^{(d)}+\Sigma^{(d)}\right)/2 \tag{5}$$

where $s,s'\in[n]$ are two input examples in the dataset, Σ is the data Gram matrix, $\partial\chi$ stands for the derivative of the activation function with respect to the pre-activation input, $N(0,M)$ stands for the mean-zero Gaussian distribution with co-variance matrix M

B Proofs of technical results

C Experimental Setup

We used standard datasets namely MNIST and CIFAR-10, with categorical cross entropy loss. We used stochastic gradient descent (SGD) and *Adam*. In the case of SGD, we tried constant step-sizes in the set $\{0.1, 0.01, 0.001\}$ and chose the best. In the case of Adam the we used a constant step size of $3e^{-4}$. In both cases, we used batch size to be 32. We used a fully connected (FC) DNN with $(w=128, d=6)$ for MNIST. To train CIFAR-10, we used *Vanilla-Convolutional* Network (VCONV) without pooling, residual connections, dropout or batch-normalisations, and is given by: input layer is $(32,32,3)$, followed by convolution layers with a stride of $(3,3)$ and channels 64, 64, 128, 128 followed by a flattening to layer with 256 hidden units, followed by a fully connected layer with 256 units, and finally a 10 width soft-max layer to produce the final predictions. To train CIFAR-10, we also used a GCONV which is same as VCONV with a *global-average-pooling* (GAP) layer. For both FRNPF, and FLNPF, we let $\chi^{\text{F}}=\chi_r$, and $G_{x,t}(l)=\gamma_r\left(q^{\text{F}}_{x,t}(l)\right)$. In the case of FRNPF, we considered two possible initialisations namely i) *independent initialisation* (II), i.e., Θ^{F}_0 and Θ_0 are statistically independent, and ii) *dependent initialisation* (DI), i.e., $\Theta^{\text{F}}_0=\Theta_0$, a case which mimics the NPFs and NPVs of a standard DNN with ReLU activations. In the case of FLNPF, $\Theta^{\text{F}}_0=\bar{\Theta}$, where $\bar{\Theta}$ is the parameter of a pre-trained (could be in various stages of training) DNN with ReLU activations. In the case, DNPFL, we let $\chi^{\text{F}}=\chi_r$, and $G_{x,t}(l)=\gamma_{sr}\left(q^{\text{F}}_{x,t}(l)\right)$ with $\beta=8$. The use of soft-ReLU makes it straightforward for the feature gradients to flow via the gating network.